```
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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2


* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS  1          Web Page for STN Seminar Schedule - N. America
 NEWS  2  AUG 15  CAOLD to be discontinued on December 31, 2008
 NEWS  3  OCT 07  EPFULL enhanced with full implementation of EPC2000
 NEWS  4  OCT 07  Multiple databases enhanced for more flexible patent
                  number searching
 NEWS  5  OCT 22  Current-awareness alert (SDI) setup and editing
                  enhanced
 NEWS  6  OCT 22  WPIDS, WPINDEX, and WPIX enhanced with Canadian PCT
                  Applications
 NEWS  7  OCT 24  CHEMLIST enhanced with intermediate list of
                  pre-registered REACH substances
 NEWS  8  NOV 21  CAS patent coverage to include exemplified prophetic
                  substances identified in English-, French-, German-,
                  and Japanese-language basic patents from 2004-present
 NEWS  9  NOV 26  MARPAT enhanced with FSORT command
 NEWS 10  NOV 26  MEDLINE year-end processing temporarily halts
                  availability of new fully-indexed citations
 NEWS 11  NOV 26  CHEMSAFE now available on STN Easy
 NEWS 12  NOV 26  Two new SET commands increase convenience of STN
                  searching
 NEWS 13  DEC 01  ChemPort single article sales feature unavailable

 NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
              AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
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 NEWS IPC8     For general information regarding STN implementation of IPC 8

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* * * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:32:48 ON 03 DEC 2008

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.21       0.21
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FILE 'REGISTRY' ENTERED AT 10:32:55 ON 03 DEC 2008

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 1 DEC 2008 HIGHEST RN 1078205-21-6
DICTIONARY FILE UPDATES: 1 DEC 2008 HIGHEST RN 1078205-21-6

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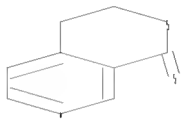
TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

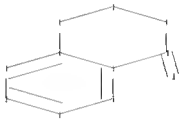
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10585029.str





chain nodes :
11
ring nodes :
1 2 3 4 5 6 7 8 9 10
chain bonds :
10-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10
exact/norm bonds :
4-7 5-10 7-8 8-9 9-10 10-11
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

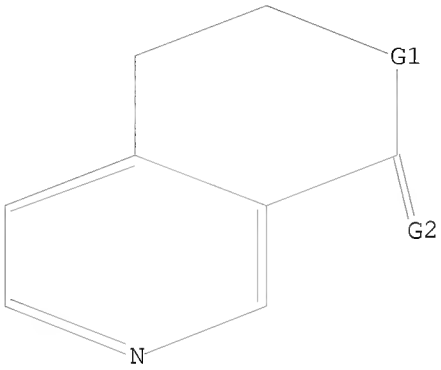
G1:O,N

G2:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 O,N

G2 O,S

Structure attributes must be viewed using STN Express query preparation.

=>

=> s l1
SAMPLE SEARCH INITIATED 10:33:28 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2990 TO ITERATE

66.9% PROCESSED 2000 ITERATIONS 11 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

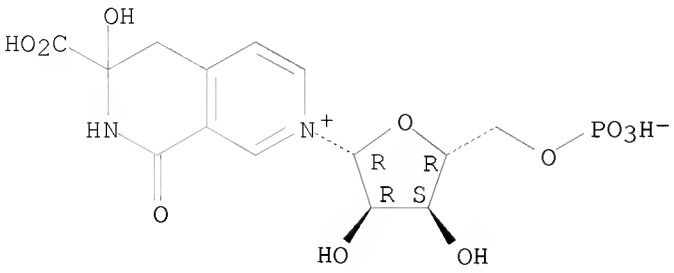
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 56521 TO 63079
PROJECTED ANSWERS: 85 TO 571

L2 11 SEA SSS SAM L1

=> d scan

L2 11 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2,7-Naphthyridinium, 3-carboxy-1,2,3,4-tetrahydro-3-hydroxy-1-oxo-7-(5-O-phosphono-β-D-ribofuranosyl)-, inner salt (9CI)
MF C14 H17 N2 O11 P

Absolute stereochemistry.



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

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=> s l1 full
FULL SEARCH INITIATED 10:33:44 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    60083 TO ITERATE

100.0% PROCESSED    60083 ITERATIONS                                 362 ANSWERS
SEARCH TIME: 00.00.01

L3          362 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     178.82     179.03

FILE 'CAPLUS' ENTERED AT 10:33:51 ON 03 DEC 2008
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FILE COVERS 1907 - 3 Dec 2008  VOL 149 ISS 23
FILE LAST UPDATED: 2 Dec 2008  (20081202/ED)

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reclassification data for the third quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s l3 full
L4          270 L3

=> file reg
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.48     179.51

FILE 'REGISTRY' ENTERED AT 10:34:01 ON 03 DEC 2008
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STRUCTURE FILE UPDATES:    1 DEC 2008  HIGHEST RN 1078205-21-6
DICTIONARY FILE UPDATES:   1 DEC 2008  HIGHEST RN 1078205-21-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.
```

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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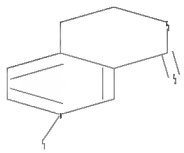
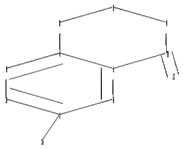
Uploading C:\Program Files\Stnexp\Queries\10585029a.str





chain nodes :
11 15
ring nodes :
1 2 3 4 5 6 7 8 9 10
chain bonds :
1-15 10-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10
exact/norm bonds :
1-15 4-7 5-10 7-8 8-9 9-10 10-11
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :
containing 1 :

G1:O,N

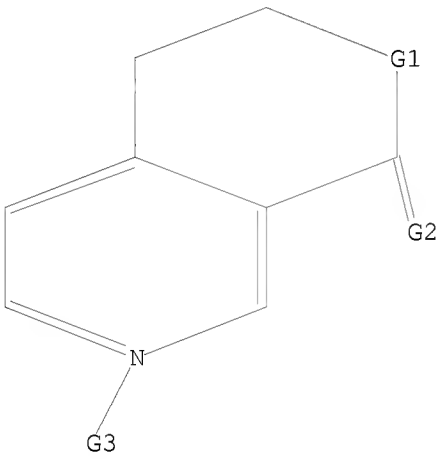
G2:O,S

G3:H,CH3

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:CLASS 15:CLASS

L5 STRUCTURE UPLOADED

=> d l5
L5 HAS NO ANSWERS
L5 STR



G1 O,N

G2 O,S

G3 H,Me

Structure attributes must be viewed using STN Express query preparation.

=> s l5 full
FULL SEARCH INITIATED 10:35:57 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 60083 TO ITERATE

100.0% PROCESSED 60083 ITERATIONS 76 ANSWERS
SEARCH TIME: 00.00.02

L6 76 SEA SSS FUL L5

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	179.28	358.79

FILE 'CAPLUS' ENTERED AT 10:36:03 ON 03 DEC 2008
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FILE COVERS 1907 - 3 Dec 2008 VOL 149 ISS 23
FILE LAST UPDATED: 2 Dec 2008 (20081202/ED)

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http://www.cas.org/legal/infopolicy.html

=> s l6 full
L7 14 L6

=> d ibib abs hitstr tot

L7 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2008:1244945 CAPLUS
DOCUMENT NUMBER: 149:478670
TITLE: A pharmaceutical compositions containing lactone type pyridine derivatives as an effective ingredient for the prevention and treatment of ischemia
INVENTOR(S): Cho, Yong-Baik; Lee, Junwon; Yi, Jung Bum; Lee, Nam Kyu; Lee, Bong-Yong; Hwang, Ki-Chul; Lim, Soyeon; Chang, Woochul; Chung, Ji Hyung; Lee, Byung Ho; Seo, Ho Won
PATENT ASSIGNEE(S): SK Chemicals Co., Ltd., S. Korea
SOURCE: PCT Int. Appl., 72pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

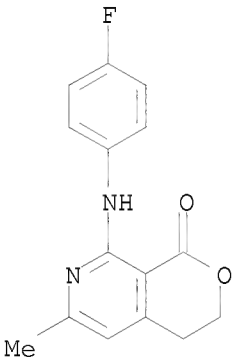
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008123756	A1	20081016	WO 2008-KR2030	20080410
W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
KR 2008091949	A	20081015	KR 2007-35075	20070410
PRIORITY APPLN. INFO.:			KR 2007-35075 A	20070410

AB The present invention relates to a pharmaceutical composition comprising a lactone type pyridine derivative for the prevention and treatment of ischemic diseases, more particularly to a pharmaceutical composition for preventing and treating ischemic diseases comprising a lactone type pyridine derivative or a pharmaceutically acceptable salt thereof as an active ingredient, which provides superior cell-protecting effect and calcium homeostasis and HSP (heat shock protein) expression controlling effect.

IT 858119-82-1, 8-(4-Fluorophenylamino)-6-methyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858119-84-3, 8-(4-Chlorophenylamino)-6-methyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858119-85-4 858119-86-5, 6-Methyl-8-p-tolylamino-3,4-dihydropyrano[3,4-c]pyridin-1-one 858119-87-6, 6-Methyl-8-phenylamino-3,4-dihydropyrano[3,4-c]pyridin-1-one 858119-88-7 858119-89-8 858119-97-8, 8-Benzylamino-6-methyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858119-99-0, 8-Amino-6-methyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-00-0 858120-01-1 858120-06-6, 8-Hydroxy-6-methyl-5-phenyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-22-6, 8-Methylamino-6-phenyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-27-1, 8-(4-Fluorophenylamino)-6-phenyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-28-2, 8-(4-Methoxybenzylamino)-6-phenyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-29-3, 8-Amino-6-phenyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-30-6 858120-31-7 858120-51-1 858120-77-1, 6-Cyclohexyl-8-(4-methoxybenzylamino)-3,4-dihydropyrano[3,4-c]pyridin-1-

one 858120-78-2, 8-Amino-6-cyclohexyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-83-9, 8-Hydroxy-6-isopropyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-86-2, 6-Isopropyl-8-(4-methoxybenzylamino)-3,4-dihydropyrano[3,4-c]pyridin-1-one 858187-08-3 1070913-29-9 1070913-32-4 1070913-33-5 1070913-35-7 1070913-45-9 1070913-48-2 1070913-52-8 1070913-53-9 1070913-54-0 1070913-55-1 1070913-56-2 1070913-57-3 1070913-58-4 1070913-59-5 1070913-60-8 1070913-79-9 1070913-80-2 1070913-81-3 1070913-82-4 1070913-97-1 1070913-98-2
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmaceutical compns. containing lactone type pyridine derivs. as an effective ingredient for prevention and treatment of ischemia)

RN 858119-82-1 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-[(4-fluorophenyl)amino]-3,4-dihydro-6-methyl- (CA INDEX NAME)



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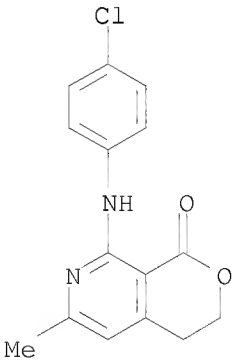

RN 858119-85-4 CAPLUS
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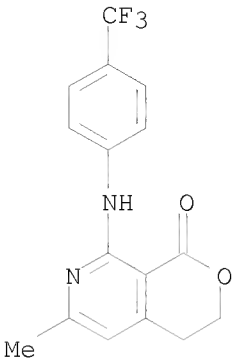

RN 858119-86-5 CAPLUS
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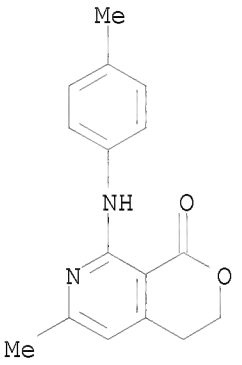

RN 858119-87-6 CAPLUS
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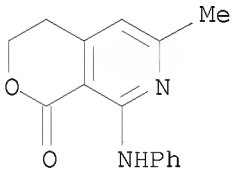

RN 858119-88-7 CAPLUS
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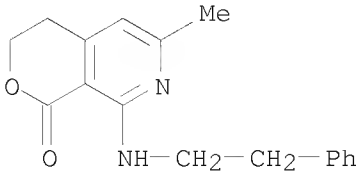

RN 858119-89-8 CAPLUS
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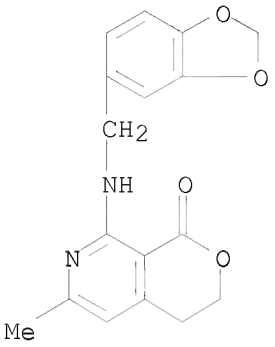

RN 858119-97-8 CAPLUS
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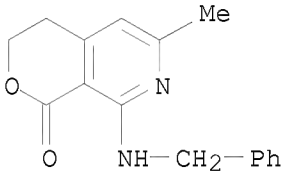

RN 858119-99-0 CAPLUS
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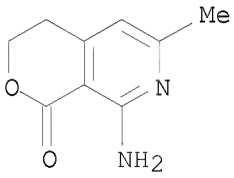

RN 858120-00-0 CAPLUS
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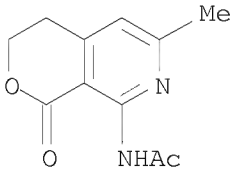

RN 858120-01-1 CAPLUS
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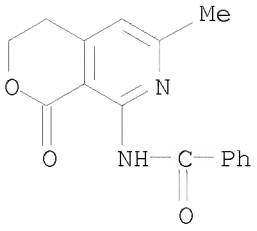

RN 858120-06-6 CAPLUS
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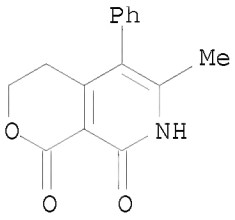
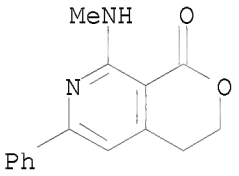
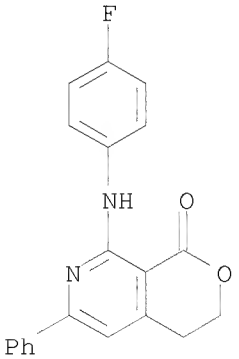


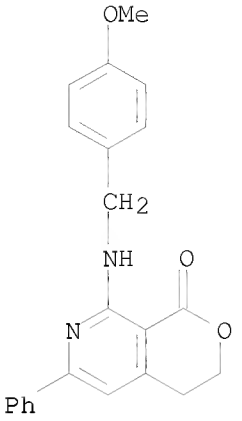
RN 858120-22-6 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-8-(methylamino)-6-phenyl- (CA INDEX NAME)



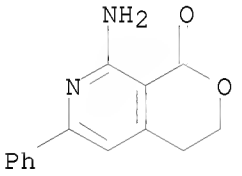
RN 858120-27-1 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-[(4-fluorophenyl)amino]-3,4-dihydro-6-phenyl- (CA INDEX NAME)



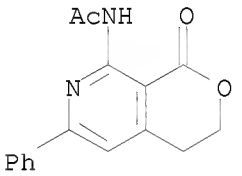
RN 858120-28-2 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-8-[[(4-methoxyphenyl)methyl]amino]-6-phenyl- (CA INDEX NAME)



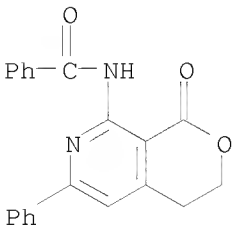
RN 858120-29-3 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-amino-3,4-dihydro-6-phenyl- (CA INDEX NAME)



RN 858120-30-6 CAPLUS
CN Acetamide, N-(3,4-dihydro-1-oxo-6-phenyl-1H-pyrano[3,4-c]pyridin-8-yl)- (CA INDEX NAME)

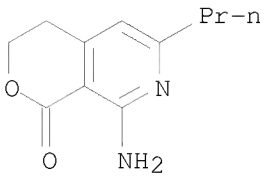


RN 858120-31-7 CAPLUS
CN Benzamide, N-(3,4-dihydro-1-oxo-6-phenyl-1H-pyrano[3,4-c]pyridin-8-yl)- (CA INDEX NAME)

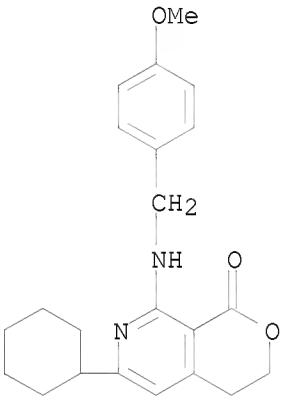


RN 858120-51-1 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-amino-3,4-dihydro-6-propyl- (CA INDEX

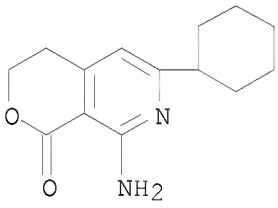
NAME)



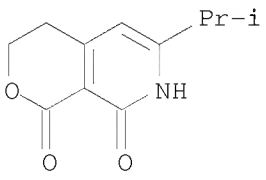
RN 858120-77-1 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 6-cyclohexyl-3,4-dihydro-8-[[(4-methoxyphenyl)methyl]amino]- (CA INDEX NAME)



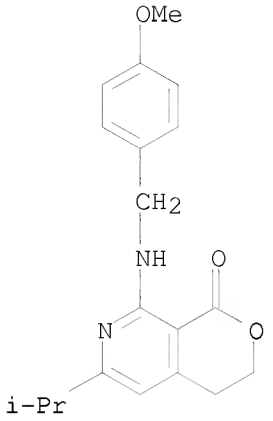
RN 858120-78-2 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-amino-6-cyclohexyl-3,4-dihydro- (CA INDEX NAME)



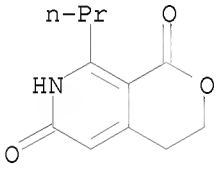
RN 858120-83-9 CAPLUS
CN 1H-Pyrano[3,4-c]pyridine-1,8(7H)-dione, 3,4-dihydro-6-(1-methylethyl)- (CA INDEX NAME)



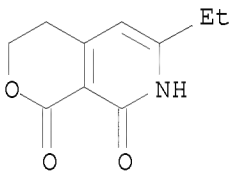
RN 858120-86-2 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-8-[[(4-methoxyphenyl)methyl]amino]-6-(1-methylethyl)- (CA INDEX NAME)



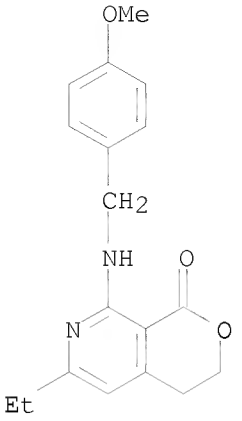
RN 858187-08-3 CAPLUS
CN 1H-Pyrano[3,4-c]pyridine-1,6(7H)-dione, 3,4-dihydro-8-propyl- (CA INDEX NAME)



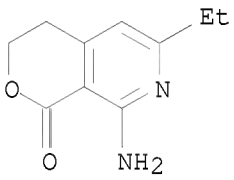
RN 1070913-29-9 CAPLUS
CN 1H-Pyrano[3,4-c]pyridine-1,8(7H)-dione, 6-ethyl-3,4-dihydro- (CA INDEX NAME)



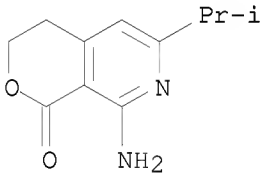
RN 1070913-32-4 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 6-ethyl-3,4-dihydro-8-[[(4-methoxyphenyl)methyl]amino]- (CA INDEX NAME)



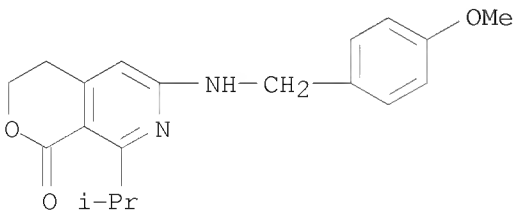
RN 1070913-33-5 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-amino-6-ethyl-3,4-dihydro- (CA INDEX NAME)



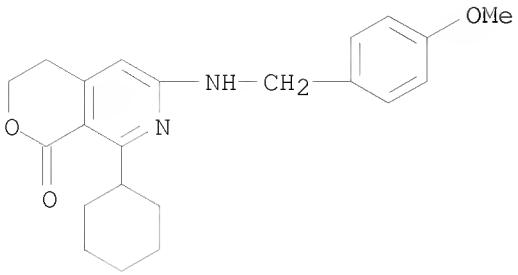
RN 1070913-35-7 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-amino-3,4-dihydro-6-(1-methylethyl)- (CA INDEX NAME)



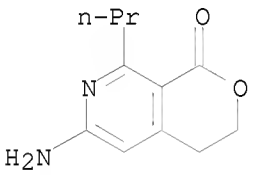
RN 1070913-45-9 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-6-[[(4-methoxyphenyl)methyl]amino]-8-(1-methylethyl)- (CA INDEX NAME)



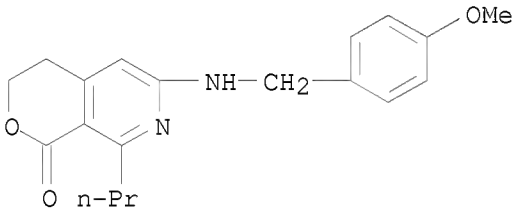
RN 1070913-48-2 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-cyclohexyl-3,4-dihydro-6-[[(4-methoxyphenyl)methyl]amino]- (CA INDEX NAME)



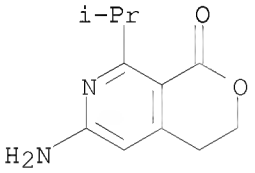
RN 1070913-52-8 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 6-amino-3,4-dihydro-8-propyl- (CA INDEX NAME)



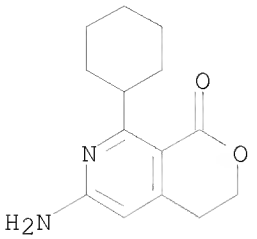
RN 1070913-53-9 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-6-[[(4-methoxyphenyl)methyl]amino]-8-propyl- (CA INDEX NAME)



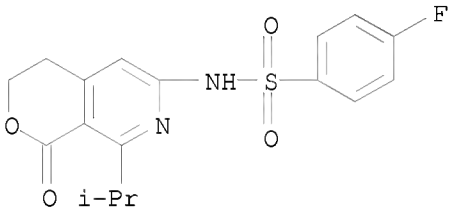
RN 1070913-54-0 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 6-amino-3,4-dihydro-8-(1-methylethyl)- (CA INDEX NAME)



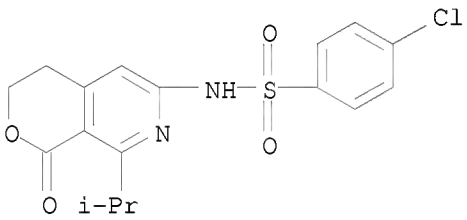
RN 1070913-55-1 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 6-amino-8-cyclohexyl-3,4-dihydro- (CA INDEX NAME)



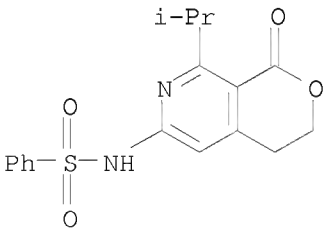
RN 1070913-56-2 CAPLUS
CN Benzenesulfonamide, N-[3,4-dihydro-8-(1-methylethyl)-1-oxo-1H-pyrano[3,4-c]pyridin-6-yl]-4-fluoro- (CA INDEX NAME)



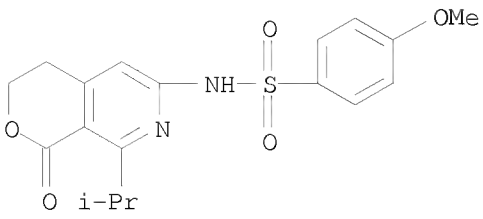
RN 1070913-57-3 CAPLUS
CN Benzenesulfonamide, 4-chloro-N-[3,4-dihydro-8-(1-methylethyl)-1-oxo-1H-pyrano[3,4-c]pyridin-6-yl]- (CA INDEX NAME)



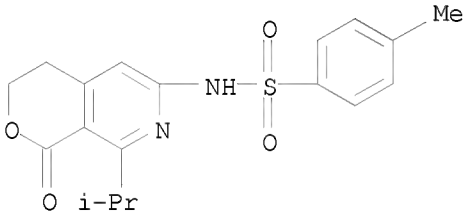
RN 1070913-58-4 CAPLUS
CN Benzenesulfonamide, N-[3,4-dihydro-8-(1-methylethyl)-1-oxo-1H-pyrano[3,4-c]pyridin-6-yl]- (CA INDEX NAME)



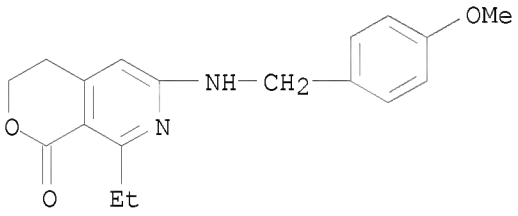
RN 1070913-59-5 CAPLUS
CN Benzenesulfonamide, N-[3,4-dihydro-8-(1-methylethyl)-1-oxo-1H-pyrano[3,4-c]pyridin-6-yl]-4-methoxy- (CA INDEX NAME)



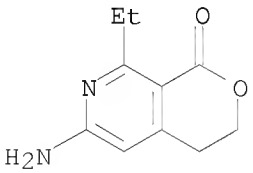
RN 1070913-60-8 CAPLUS
CN Benzenesulfonamide, N-[3,4-dihydro-8-(1-methylethyl)-1-oxo-1H-pyrano[3,4-c]pyridin-6-yl]-4-methyl- (CA INDEX NAME)



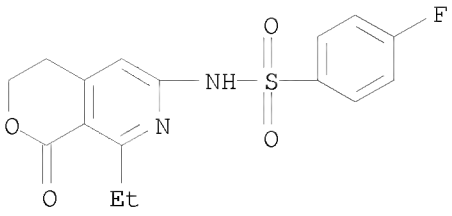
RN 1070913-79-9 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-ethyl-3,4-dihydro-6-[[(4-methoxyphenyl)methyl]amino]- (CA INDEX NAME)



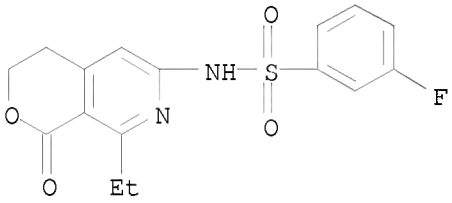
RN 1070913-80-2 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 6-amino-8-ethyl-3,4-dihydro- (CA INDEX NAME)



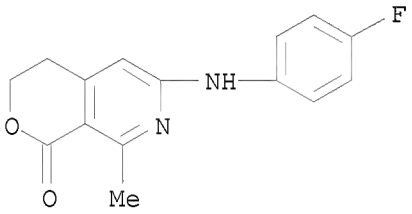
RN 1070913-81-3 CAPLUS
CN Benzenesulfonamide, N-(8-ethyl-3,4-dihydro-1-oxo-1H-pyrano[3,4-c]pyridin-6-yl)-4-fluoro- (CA INDEX NAME)



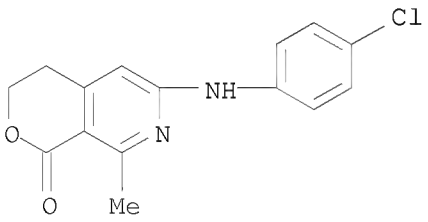
RN 1070913-82-4 CAPLUS
CN Benzenesulfonamide, N-(8-ethyl-3,4-dihydro-1-oxo-1H-pyrano[3,4-c]pyridin-6-yl)-3-fluoro- (CA INDEX NAME)



RN 1070913-97-1 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 6-[(4-fluorophenyl)amino]-3,4-dihydro-8-methyl- (CA INDEX NAME)



RN 1070913-98-2 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 6-[(4-chlorophenyl)amino]-3,4-dihydro-8-methyl- (CA INDEX NAME)



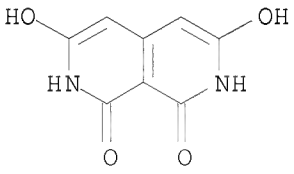
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:262396 CAPLUS
DOCUMENT NUMBER: 146:481960
TITLE: A Novel Lumazine Synthase Inhibitor Derived from Oxidation of 1,3,6,8-Tetrahydroxy-2,7-naphthyridine to a Tetraazaperylenehexaone Derivative
AUTHOR(S): Zhang, Yanlei; Illarionov, Boris; Bacher, Adelbert; Fischer, Markus; Georg, Gunda I.; Ye, Qi-Zhuang; Vander Velde, David; Fanwick, Phillip E.; Song, Yunlong; Cushman, Mark
CORPORATE SOURCE: Department of Medicinal Chemistry and Molecular Pharmacology, School of Pharmacy and Pharmaceutical Sciences, and The Purdue Cancer Center, Purdue University, West Lafayette, IN, 47907, USA
SOURCE: Journal of Organic Chemistry (2007), 72(8), 2769-2776
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:481960

AB Air oxidation of 1,3,6,8-tetrahydroxy-2,7-naphthyridine afforded 2,5,8,11-tetraaza-5,11-dihydro-4,10-dihydroxyperylene-1,3,6,7,9,12-hexaone. X-Ray crystallog. of the product revealed that it exists in the meso form in the solid state. The mechanism of product formation most likely involves oxidative phenolic coupling and oxidation The product proved to be a competitive inhibitor of Schizosaccharomyces pombe lumazine synthase with a Ki of 66 ± 13 μM in Tris buffer and 22 ± 4 μM in phosphate buffer. This is significantly more potent than the naphthyridine reactant (Ki 350 ± 76 μM, competitive inhibition), which had previously been identified as a lumazine synthase inhibitor by high-throughput screening. Ab initio calcns. indicate that the meso form is slightly less stable than the enantiomeric form, and that the two forms interconvert rapidly at room temperature

IT 53162-08-6P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tetraazaperylenehexaone by aerial oxidation of tetrahydroxynaphthyridine as lumazine synthase inhibitor and its conformational and mol. docking studies)

RN 53162-08-6 CAPLUS
CN 2,7-Naphthyridine-1,8(2H,7H)-dione, 3,6-dihydroxy- (CA INDEX NAME)

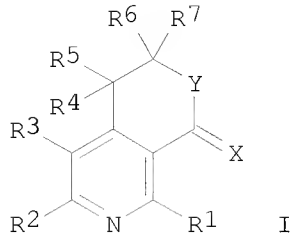


REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

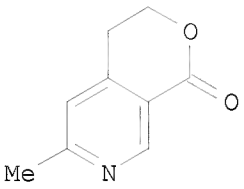
L7 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:612303 CAPLUS
DOCUMENT NUMBER: 143:133284
TITLE: Preparation of pyridines as inhibitors of cytokine production and pharmaceutical compositions containing them useful in the treatment of pain and inflammatory and immune diseases
INVENTOR(S): Kim, Hyung Ook; Lee, Nam Kyu; Kim, Joo Hyon; Rhee, Hae In; Cho, Yong-Baik; Ryu, Je Ho; Kim, Nam Ho; Ryu, Keun Ho; Yi, Jung Bum; Jung, Jae Yoon
PATENT ASSIGNEE(S): SK Chemicals, Co. Ltd., S. Korea
SOURCE: PCT Int. Appl., 119 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2005063768	A1	20050714	WO 2004-KR3545		20041230
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2004309303	A1	20050714	AU 2004-309303		20041230
CA 2552207	A1	20050714	CA 2004-2552207		20041230
EP 1706412	A1	20061004	EP 2004-808673		20041230
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS					
CN 1938315	A	20070328	CN 2004-80041948		20041230
BR 2004018301	A	20070502	BR 2004-18301		20041230
JP 2007517024	T	20070628	JP 2006-546849		20041230
IN 2006DN03779	A	20070622	IN 2006-DN3779		20060630
US 20070254909	A1	20071101	US 2007-585029		20070416
PRIORITY APPLN. INFO.:			KR 2003-100132	A	20031230
			WO 2004-KR3545	W	20041230

OTHER SOURCE(S): CASREACT 143:133284; MARPAT 143:133284
GI



I



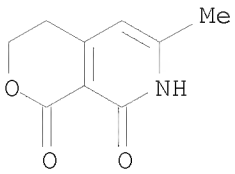
II

AB The invention is related to novel pyridine derivs. I [wherein R1-R7 = independently H, halo, CN, NO2, acyl, OH, low alkyl, etc.; X = O, S; Y = O, NH and derivs.] and their pharmaceutically acceptable salts having an inhibitory effect on production of cytokines, which are involved in inflammatory responses, and being used as antiinflammatory and analgesic agents. For example, II was prepared by cyclization of 4-(2-hydroxyethyl)-6-methylnicotinonitrile (preparation given) in the presence of concentrated HCl. I showed excellent inhibitory effects on the production of TNF-α, IL-1α, IL-6, INF-γ, PGE2. I have shown superiorities in antiinflammatory and analgesic effects over Indomethacin and Celecoxib. Thus, I are useful for treating inflammation and immune diseases.

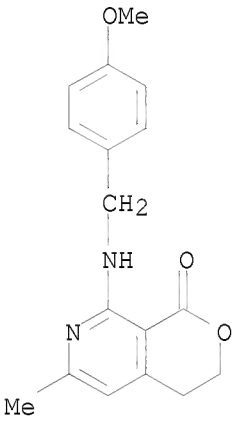
IT 858119-67-2P, 8-Hydroxy-6-methyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858119-98-9P 858119-99-0P, 8-Amino-6-methyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-15-7P, 8-Hydroxy-6-phenyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-28-2P, 8-(4-Methoxybenzylamino)-6-phenyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-29-3P, 8-Amino-6-phenyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-43-1P, 8-Hydroxy-6-propyl-3,4-dihydropyrano[3,4-c]pyridin-1-one hydrochloride 858120-44-2P, 6-Hydroxy-8-propyl-3,4-dihydropyrano[3,4-c]pyridin-1-one hydrochloride 858120-50-0P, 8-(4-Methoxybenzylamino)-6-(n-propyl)-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-51-1P, 8-Amino-6-(n-propyl)-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-73-7P, 6-Cyclohexyl-8-hydroxy-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-77-1P, 6-Cyclohexyl-8-(4-methoxybenzylamino)-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-83-9P, 8-Hydroxy-6-isopropyl-3,4-dihydropyrano[3,4-c]pyridin-1-one
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of cytokine production-inhibiting pyridine derivs.
useful in treating pain and inflammatory and immune diseases)

RN 858119-67-2 CAPLUS

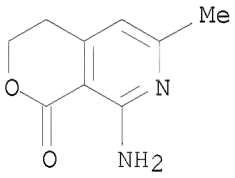
CN 1H-Pyrano[3,4-c]pyridine-1,8(7H)-dione, 3,4-dihydro-6-methyl- (CA INDEX NAME)



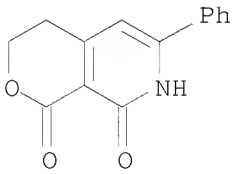
RN 858119-98-9 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-8-[[(4-methoxyphenyl)methyl]amino]-6-methyl- (CA INDEX NAME)



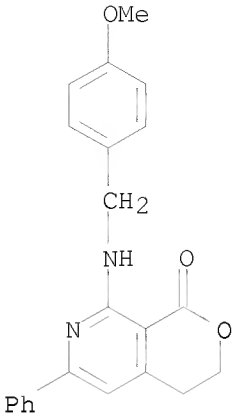
RN 858119-99-0 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-amino-3,4-dihydro-6-methyl- (CA INDEX NAME)



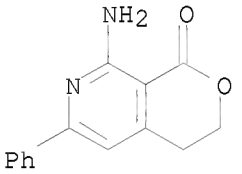
RN 858120-15-7 CAPLUS
CN 1H-Pyrano[3,4-c]pyridine-1,8(7H)-dione, 3,4-dihydro-6-phenyl- (CA INDEX NAME)



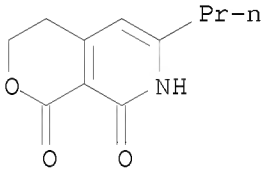
RN 858120-28-2 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-8-[[(4-methoxyphenyl)methyl]amino]-6-phenyl- (CA INDEX NAME)



RN 858120-29-3 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-amino-3,4-dihydro-6-phenyl- (CA INDEX NAME)

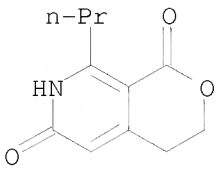


RN 858120-43-1 CAPLUS
CN 1H-Pyrano[3,4-c]pyridine-1,8(7H)-dione, 3,4-dihydro-6-propyl-, hydrochloride (1:1) (CA INDEX NAME)



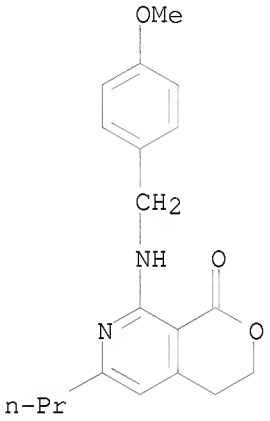
● HCl

RN 858120-44-2 CAPLUS
CN 1H-Pyrano[3,4-c]pyridine-1,6(7H)-dione, 3,4-dihydro-8-propyl-, hydrochloride (1:1) (CA INDEX NAME)

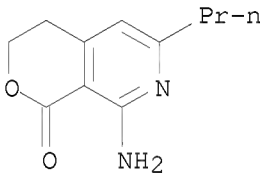


● HCl

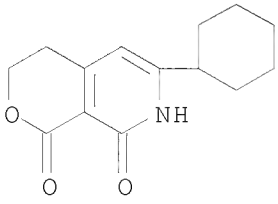
RN 858120-50-0 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-8-[[(4-methoxyphenyl)methyl]amino]-6-propyl- (CA INDEX NAME)



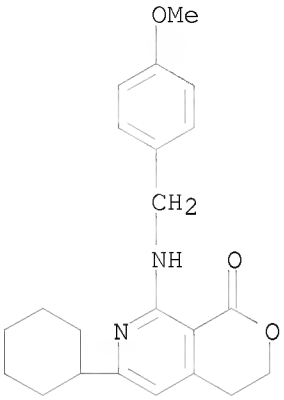
RN 858120-51-1 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-amino-3,4-dihydro-6-propyl- (CA INDEX NAME)



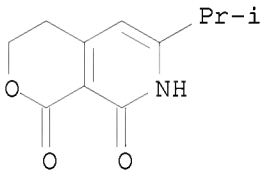
RN 858120-73-7 CAPLUS
CN 1H-Pyrano[3,4-c]pyridine-1,8(7H)-dione, 6-cyclohexyl-3,4-dihydro- (CA INDEX NAME)



RN 858120-77-1 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 6-cyclohexyl-3,4-dihydro-8-[[(4-methoxyphenyl)methyl]amino]- (CA INDEX NAME)



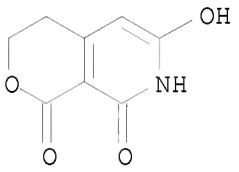
RN 858120-83-9 CAPLUS
CN 1H-Pyrano[3,4-c]pyridine-1,8(7H)-dione, 3,4-dihydro-6-(1-methylethyl)- (CA INDEX NAME)



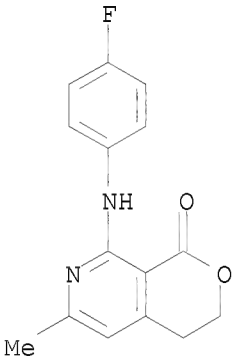
IT 858119-64-9P, 6,8-Dihydroxy-3,4-dihydropyrano[3,4-c]pyridin-1-one 858119-82-1P, 8-(4-Fluorophenylamino)-6-methyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858119-84-3P, 8-(4-Chlorophenylamino)-6-methyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858119-85-4P, 8-[(4-Trifluoromethylphenyl)amino]-6-methyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858119-86-5P, 6-Methyl-8-(p-tolylamino)-3,4-dihydropyrano[3,4-c]pyridin-1-one 858119-87-6P, 6-Methyl-8-phenylamino-3,4-dihydropyrano[3,4-c]pyridin-1-one 858119-88-7P, 6-Methyl-8-[(2-phenylethyl)amino]-3,4-dihydropyrano[3,4-c]pyridin-1-one 858119-89-8P, 8-[(Benzodioxol-5-ylmethyl)amino]-6-methyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858119-97-8P, 8-Benzylamino-6-methyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-00-0P, 8-Acetamido-6-methyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-01-1P, N-(1-Oxo-6-methyl-3,4-dihydropyrano[3,4-c]pyridin-8-yl)benzamide 858120-06-6P, 8-Hydroxy-6-methyl-5-phenyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-22-6P, 8-Methylamino-6-phenyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-27-1P, 8-(4-Fluorophenylamino)-6-phenyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-30-6P, 8-Acetamido-6-phenyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-31-7P, N-(1-Oxo-6-phenyl-3,4-dihydropyrano[3,4-c]pyridin-8-yl)benzamide 858120-34-0P, 6-Hydroxy-8-methyl-3,4-dihydropyrano[3,4-c]pyridin-1-one hydrochloride 858120-52-2P, N-[1-Oxo-6-(n-propyl)-3,4-dihydro-1H-pyrano[3,4-c]pyridin-8-yl]acetamide 858120-78-2P, 8-Amino-6-cyclohexyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-86-2P, 6-Isopropyl-8-(4-methoxybenzylamino)-3,4-

dihydropyrano[3,4-c]pyridin-1-one 858120-87-3P,
6-Hydroxy-8-methyl-3,4-dihydropyrano[3,4-c]pyridin-1-one
858120-88-4P, 8-Hydroxy-6-(n-propyl)-3,4-dihydropyrano[3,4-
c]pyridin-1-one
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(drug candidate; preparation of cytokine production-inhibiting pyridine
derivs.
useful in treating pain and inflammatory and immune diseases)

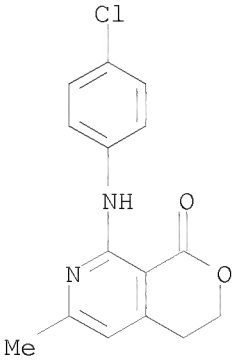
RN 858119-64-9 CAPLUS
CN 1H-Pyrano[3,4-c]pyridine-1,6(7H)-dione, 3,4-dihydro-8-hydroxy- (CA INDEX NAME)



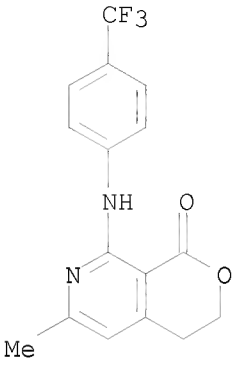
RN 858119-82-1 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-[(4-fluorophenyl)amino]-3,4-dihydro-6-methyl- (CA INDEX NAME)



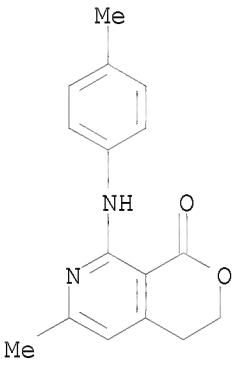
RN 858119-84-3 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-[(4-chlorophenyl)amino]-3,4-dihydro-6-methyl- (CA INDEX NAME)



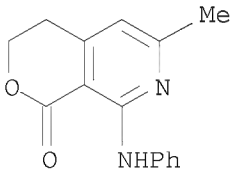
RN 858119-85-4 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-6-methyl-8-[[4-(trifluoromethyl)phenyl]amino]- (CA INDEX NAME)



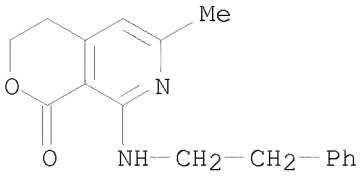
RN 858119-86-5 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-6-methyl-8-[(4-methylphenyl)amino]- (CA INDEX NAME)



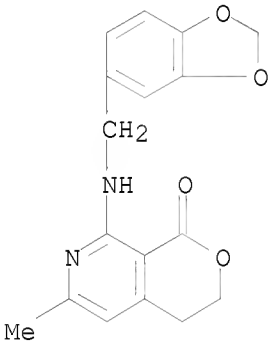
RN 858119-87-6 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-6-methyl-8-(phenylamino)- (CA INDEX NAME)



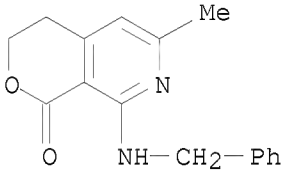
RN 858119-88-7 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-6-methyl-8-[(2-phenylethyl)amino]- (CA INDEX NAME)



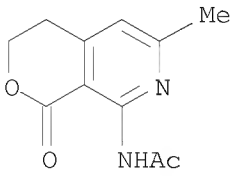
RN 858119-89-8 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-[(1,3-benzodioxol-5-ylmethyl)amino]-3,4-dihydro-6-methyl- (CA INDEX NAME)



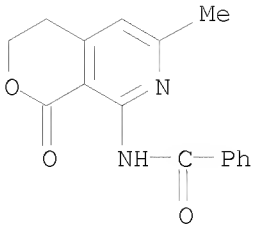
RN 858119-97-8 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-6-methyl-8-[(phenylmethyl)amino]- (CA INDEX NAME)



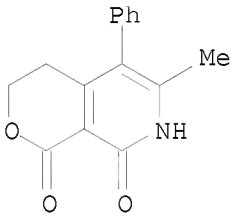
RN 858120-00-0 CAPLUS
CN Acetamide, N-(3,4-dihydro-6-methyl-1-oxo-1H-pyrano[3,4-c]pyridin-8-yl)- (CA INDEX NAME)



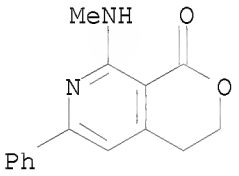
RN 858120-01-1 CAPLUS
CN Benzamide, N-(3,4-dihydro-6-methyl-1-oxo-1H-pyrano[3,4-c]pyridin-8-yl)- (CA INDEX NAME)



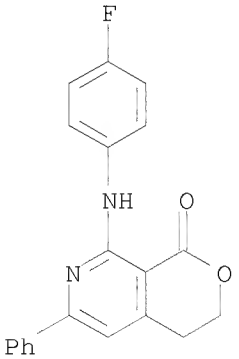
RN 858120-06-6 CAPLUS
CN 1H-Pyrano[3,4-c]pyridine-1,8(7H)-dione, 3,4-dihydro-6-methyl-5-phenyl- (CA INDEX NAME)



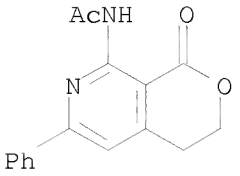
RN 858120-22-6 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-8-(methylamino)-6-phenyl- (CA INDEX NAME)



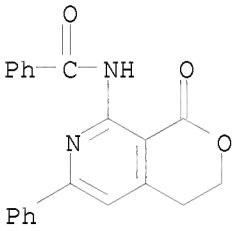
RN 858120-27-1 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-[(4-fluorophenyl)amino]-3,4-dihydro-6-phenyl- (CA INDEX NAME)



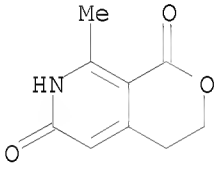
RN 858120-30-6 CAPLUS
CN Acetamide, N-(3,4-dihydro-1-oxo-6-phenyl-1H-pyrano[3,4-c]pyridin-8-yl)- (CA INDEX NAME)



RN 858120-31-7 CAPLUS
CN Benzamide, N-(3,4-dihydro-1-oxo-6-phenyl-1H-pyrano[3,4-c]pyridin-8-yl)-
(CA INDEX NAME)

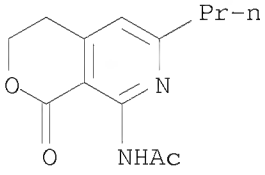


RN 858120-34-0 CAPLUS
CN 1H-Pyrano[3,4-c]pyridine-1,6(7H)-dione, 3,4-dihydro-8-methyl-,
hydrochloride (1:1) (CA INDEX NAME)

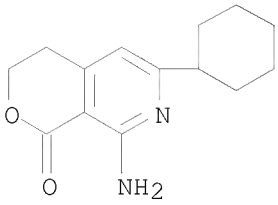


● HCl

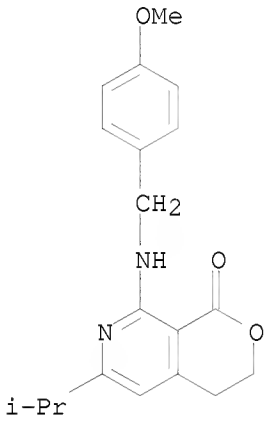
RN 858120-52-2 CAPLUS
CN Acetamide, N-(3,4-dihydro-1-oxo-6-propyl-1H-pyrano[3,4-c]pyridin-8-yl)-
(CA INDEX NAME)



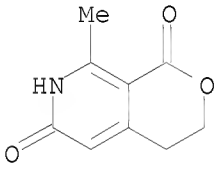
RN 858120-78-2 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-amino-6-cyclohexyl-3,4-dihydro- (CA
INDEX NAME)



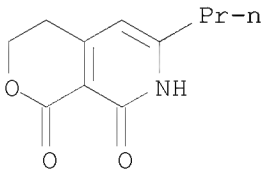
RN 858120-86-2 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-8-[[(4-methoxyphenyl)methyl]amino]-6-(1-methylethyl)- (CA INDEX NAME)



RN 858120-87-3 CAPLUS
CN 1H-Pyrano[3,4-c]pyridine-1,6(7H)-dione, 3,4-dihydro-8-methyl- (CA INDEX NAME)



RN 858120-88-4 CAPLUS
CN 1H-Pyrano[3,4-c]pyridine-1,8(7H)-dione, 3,4-dihydro-6-propyl- (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

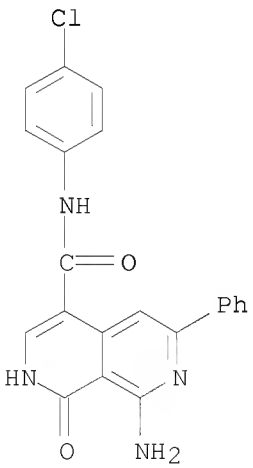
L7 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:41677 CAPLUS
DOCUMENT NUMBER: 138:337967
TITLE: Studies with alkylheterocycles: novel synthesis of functionally substituted isoquinoline and pyridopyridine derivatives
AUTHOR(S): Elmaati, Tarek M. Abu; El-Taweel, Fathy M. A.
CORPORATE SOURCE: Faculty of Specific Education, New Damietta, Mansoura University, Egypt
SOURCE: Journal of the Chinese Chemical Society (Taipei, Taiwan) (2002), 49(6), 1045-1050
CODEN: JCCTAC; ISSN: 0009-4536
PUBLISHER: Chinese Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:337967
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

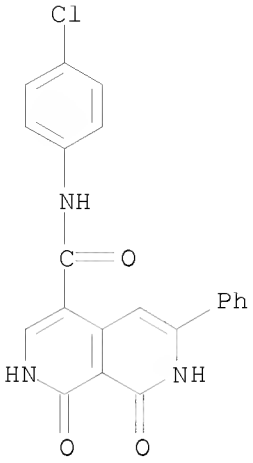
AB Reaction of cyanopyridinone I with cinnamonitriles gave isoquinolines such as II [R = (un)substituted phenyl]. Treating I with elemental sulfur yielded thienopyridine III. III reacted with acrylonitrile to give isoquinoline II (R = H). II (R = H) was also prepared from I and methylenemalononitrile. Condensation of I with benzaldehyde, followed by treatment with NH4OH or AcOH/HCl gave pyridopyridine IV or V.

IT 517907-24-3P 517907-25-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(conversion of cyanopyridinone derivative to isoquinolinones, thienopyridinone, and pyridopyridines by reactions with unsatd. nitriles, sulfur, or benzaldehyde)

RN 517907-24-3 CAPLUS
CN 2,7-Naphthyridine-4-carboxamide, 8-amino-N-(4-chlorophenyl)-1,2-dihydro-1-oxo-6-phenyl- (CA INDEX NAME)



RN 517907-25-4 CAPLUS
CN 2,7-Naphthyridine-4-carboxamide, N-(4-chlorophenyl)-1,2,7,8-tetrahydro-1,8-dioxo-6-phenyl- (CA INDEX NAME)

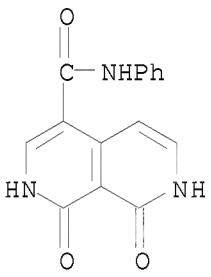


REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:501464 CAPLUS
DOCUMENT NUMBER: 137:352926
TITLE: 1-(N,N-dimethylamino)-2-(N-phenylcarbamoyl)-1-buten-3-one as a building block for the synthesis of heterocyclic compounds
AUTHOR(S): Elmaati, T. A.; Said, S.; Elenein, N. A.; Sofan, M.; Khodeir, N.
CORPORATE SOURCE: Faculty of Specific Education, Mansoura University, New Damietta, Egypt
SOURCE: Polish Journal of Chemistry (2002), 76(7), 945-952
CODEN: PJCHDQ; ISSN: 0137-5083
PUBLISHER: Polish Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:352926

AB Acetoacetanilide reacted with DMF-DMA to give the enaminone MeCOC(:CHNMe2)CONHPh (I). I, when treated with hydrazines, gives pyrazoles, resp., and with pyrazole derivs. the pyrazolopyrimidines. On the other hand, in reaction of I with benzimidazole and benzimidazole-2-acetonitrile, pyrimidobenzimidazole and the pyridobenzimidazole were formed. I reacts with hippuric acid in boiling acetic anhydride to afford a pyridine derivative In the reaction of I with malononitrile, cyanoacetamide or malononitrile dimer compds. were formed.

IT 474369-52-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(use of (N,N-dimethylamino)(N-phenylcarbamoyl)butenone as a building block for the synthesis of heterocyclic compds.)
RN 474369-52-3 CAPLUS
CN 2,7-Naphthyridine-4-carboxamide, 1,2,7,8-tetrahydro-1,8-dioxo-N-phenyl- (CA INDEX NAME)

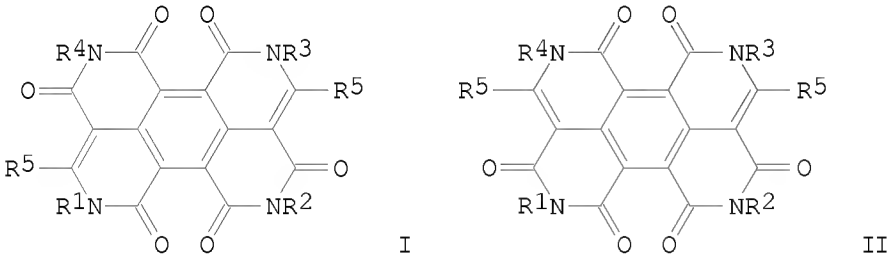


REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:61571 CAPLUS
DOCUMENT NUMBER: 116:61571
ORIGINAL REFERENCE NO.: 116:10627a,10630a
TITLE: Heterocyclic compounds and their use as dyes and pigments
INVENTOR(S): Hoechstetter, Hans
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 18 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3937633	A1	19910516	DE 1989-3937633	19891111
US 5097027	A	19920317	US 1990-593460	19901005
EP 427993	A2	19910522	EP 1990-120651	19901027
EP 427993	A3	19920122		
R: CH, DE, FR, GB, LI				
JP 03181567	A	19910807	JP 1990-299089	19901106

PRIORITY APPLN. INFO.: DE 1989-3937633 A 19891111
OTHER SOURCE(S): MARPAT 116:61571
GI



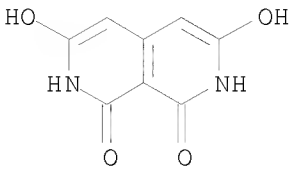
I II

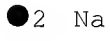
AB The dyes and pigments are I and II (R1-R4 = H, alkyl, cycloalkyl, aryl, aralkyl, heteroaryl; R5 = halogen, NR1R2, SR1, OR1, aryl, heteroaryl, OX; X = cation; when R-R4 = H, R5 ≠ OH, ONa). Thus, 29 g 2,7-naphthyridine-1,3,6,8-tetraol di-Na salt in 90 mL MeC6H4SO3Me was heated 12.5 h at 190°, cooled to 100°, and precipitated in MeOH to give 23 g I-II mixture (R1-R4 = Me; R5 = OH) (III). III was a reddish violet pigment with good migration resistance.

IT 137219-69-3
RL: USES (Uses)
(alkylation-dimerization of, in manufacture of pigments and dyes)

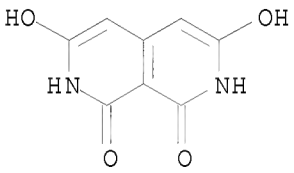
RN 137219-69-3 CAPLUS

CN 2,7-Naphthyridine-1,8(2H,7H)-dione, 3,6-dihydroxy-, sodium salt (1:2) (CA INDEX NAME)

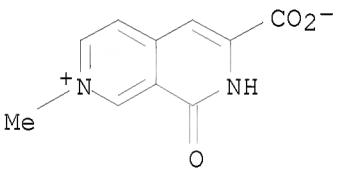

HO
OH
HN
NH
O
O


2 Na

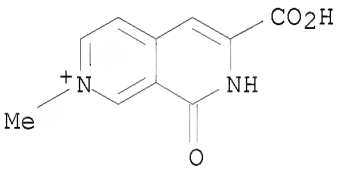
L7 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1974:437490 CAPLUS
DOCUMENT NUMBER: 81:37490
ORIGINAL REFERENCE NO.: 81:6003a,6006a
TITLE: Condensation of dicarbonyl compounds with malononitrile. VIII. Condensation of malononitrile with some esters of β-keto acids
AUTHOR(S): Gudriniece, E.; Rigerte, B.
CORPORATE SOURCE: Rizh. Politekh. Inst., Riga, USSR
SOURCE: Latvijas PSR Zinatnu Akademijas Vestis, Kimijas Serija (1974), (2), 239-40
CODEN: LZAKAM; ISSN: 0002-3248
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB Nicotinonitriles I (R = Me, Ph) were obtained in 56% and 20% yields, resp., by condensing malononitrile with RCOCH2CO2Et to give intermediate RC(CH2CO2Et):C(CN)2 which were cyclized by 70% HClO4. Analogously obtained was 77% naphthyridine II from malononitrile and (EtO2CCH2)2CO.
IT 53162-08-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 53162-08-6 CAPLUS
CN 2,7-Naphthyridine-1,8(2H,7H)-dione, 3,6-dihydroxy- (CA INDEX NAME)



L7 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1973:466219 CAPLUS
DOCUMENT NUMBER: 79:66219
ORIGINAL REFERENCE NO.: 79:10699a,10702a
TITLE: Simple synthesis of 1-hydroxy-3-naphthyridinecarboxylic acid
AUTHOR(S): Trommer, Wolfgang; Blume, Heinrich
CORPORATE SOURCE: Abt. Chem., Ruhr Univ., Bochum, Fed. Rep. Ger.
SOURCE: Tetrahedron Letters (1973), (17), 1447-8
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB Condensation of 3-cyano-4-methylpyridine (prepared by heating the 3-bromo analog with CuCN) with (CO2Et)2 using Me3COK as base gave the cyano ester (I) which gave the title compound (II) on hydrolysis. The 7-Me analog of II was prepared in 80% yield by 1,4-addition of MeCOCO2H to N-methylnicotinamide chloride followed by oxidation with p-ONC6H4NMe2 or (Cl3C)2CO.
IT 42285-32-5P 42285-33-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 42285-32-5 CAPLUS
CN 2,7-Naphthyridinium, 6-carboxy-7,8-dihydro-2-methyl-8-oxo-, inner salt (CA INDEX NAME)



RN 42285-33-6 CAPLUS
CN 2,7-Naphthyridinium, 6-carboxy-7,8-dihydro-2-methyl-8-oxo-, chloride (1:1) (CA INDEX NAME)



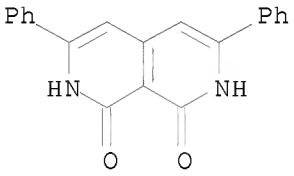
● Cl−

L7 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1970:435253 CAPLUS
DOCUMENT NUMBER: 73:35253
ORIGINAL REFERENCE NO.: 73:5841a,5844a
TITLE: Reactions of some 4-methylene-4H-pyran derivatives with primary and secondary amines
AUTHOR(S): Van Allan, James A.; Reynolds, George Arthur; Petropoulos, C. C.; Maier, D. P.
CORPORATE SOURCE: Res. Lab., Eastman Kodak Co., Rochester, NY, USA
SOURCE: Journal of Heterocyclic Chemistry (1970), 7(3), 495-507
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 73:35253

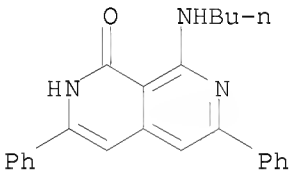
AB 4-Dicyanomethylene-4H-pyrans react with secondary amines to give 2-aminopyridine and 2-pyridone derivs., which, in turn, were used to prepare copyrine derivatives. These pyrans and pyrimary amines gave copyrine and iminopyridone derivatives in addition to dicyanomethylene-1,4-dihydropyridines. Reaction of cyanocarbamoylmethylene-4H-pyrans with secondary amines gave 2-pyrones, and with primary amines, gave copyrines and 1,4-dihydropyridine derivs.

IT 27337-84-4P 27337-98-0P 27338-00-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

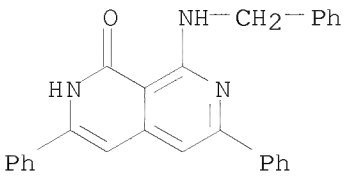
RN 27337-84-4 CAPLUS
CN 2,7-Naphthyridine-1,8(2H,7H)-dione, 3,6-diphenyl- (CA INDEX NAME)



RN 27337-98-0 CAPLUS
CN 2,7-Naphthyridin-1(2H)-one, 8-(butylamino)-3,6-diphenyl- (CA INDEX NAME)



RN 27338-00-7 CAPLUS
CN 2,7-Naphthyridin-1(2H)-one, 3,6-diphenyl-8-[(phenylmethyl)amino]- (CA INDEX NAME)

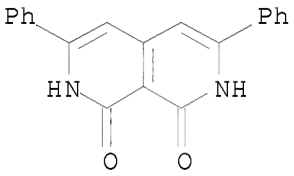


L7 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1966:11376 CAPLUS
DOCUMENT NUMBER: 64:11376
ORIGINAL REFERENCE NO.: 64:2046c-d
TITLE: Condensations of carbonyl compounds at the methyl or α-methylene group of 6- or 4-alkyl-3-cyano-2(1)-pyridones through dianions
AUTHOR(S): Boatman, Sandra; Harris, Thomas M.; Hauser, Charles R.
CORPORATE SOURCE: Duke Univ., Durham, NC
SOURCE: Journal of the American Chemical Society (1965), 87(22), 5198-202
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 64:11376

AB Several types of condensations of carbonyl compds. at the methyl or methylene group of 6- or 4-alkyl-3-cyano-2(1)-pyridones were effected through dianions, which were prepared by means of 2 mole-equivs. of potassium amide in liquid ammonia. The types of condensations realized were aroylation with methyl benzoate, acylation with ethyl oxalate, carbonyl addition with benzophenone or benzaldehyde, and conjugate addition with chalcone. One of the benzoyl derivs. was converted by polyphosphoric acid to the corresponding amide and another to a dihydroxy-2,7-naphthyridine. The carbonyl addition products were dehydrated or converted to another derivative Consideration is given to possible extensions of the method.

IT 27337-84-4P, 2,7-Naphthyridine-1,8-diol, 3,6-diphenyl-
RL: PREP (Preparation)
(preparation of)

RN 27337-84-4 CAPLUS
CN 2,7-Naphthyridine-1,8(2H,7H)-dione, 3,6-diphenyl- (CA INDEX NAME)

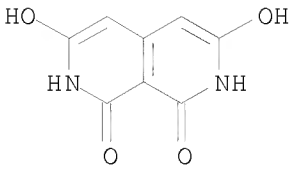


L7 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1961:13414 CAPLUS
DOCUMENT NUMBER: 55:13414
ORIGINAL REFERENCE NO.: 55:2640b-f
TITLE: Some derivatives of 2,7-naphthyridine
AUTHOR(S): Ferrier, B. M.; Campbell, Neil
CORPORATE SOURCE: Univ. Edinburgh, UK
SOURCE: Journal of the Chemical Society (1960) 3513-15
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

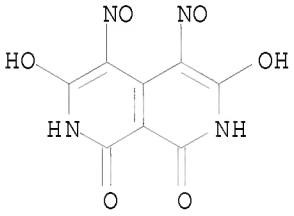
AB The synthesis of some 2,7-naphthyridine derivs. was described. $CH_2(CN)_2$ (1 g.) kept 19 days with 3 g. $CO(CH_2CO_2Et)_2$ in 25 ml. alc. containing 4 drops $NHEt_2$ gave 2.6 g. di-Et β-(dicyanomethylene)glutarate, yellow needles, m. 166° (C_6H_6). $CH_2(CN)_2$ (1.1 g.) was condensed with $CO(CH_2CO_2Et)_2$ as above; after 24 hrs. no ketone could be detected and after a further 24 hrs. the solvent removed, the residue warmed 30 sec. with 20 ml. 70% H_2SO_4, then refluxed 30 sec., cooled, and poured into 60 ml. H_2O gave 2.7 g. 1,3,6,8-tetrahydroxy-2,7-naphthyridine (I), m. above 350°; dibenzoate m. 234-9°; dinitroso compound m. above 350°. I (1 g.) heated 24 hrs. at 180° in a sealed tube with 10 ml. $POCl_3$, the mixture poured on 150 g. ice, made alkaline, and extracted with Et_2O gave 0.5 g. 1,3,6,8-tetrachloro-2,7-naphthyridine (II), yellow needles, m. 157-61° (aqueous alc.). The residue after extraction with ligroine gave 0.1 g. 1,3,8-trichloro-8-hydroxy-2,7-naphthyridine, m. 295° (C_6H_6). II (0.46 g.), 1 g. fused KOAc, and 0.2 g. $PdCl_2$ in 40 ml. MeOH shaken with H, the oily residue dissolved in H_2O, made alkaline, and extracted with EtOAc gave 0.04 g. 1,2,3,4-tetrahydro-2,7-naphthyridine picrate, orange-yellow prisms, m. 248-50° (H_2O). II (0.36 g.), 0.2 g. $PdCl_2$, and 1 g. anhydrous K_2CO_3 in 25 ml. MeOH shaken 1 hr. with H gave 0.014 g. 1,8-dimethoxy-2,7-naphthyridine, m. 108-10°; picrate, yellow blades, m. 148-50° (C_6H_6). From the MeOH filtrate tetrahydro-2,7-naphthyridine was isolated as the picrate. II (0.1 g.) in 5 ml. MeOH with 0.1 g. anhydrous K_2CO_3 afforded after 1 hr. 3,6-dichloro-1,8-dimethoxy-2,7-naphthyridine (III), needles, m. 155-7° (MeOH). III (0.08 g.) was obtained when 0.1 g. II was refluxed 1 hr. in 5 ml. MeOH with 5 ml. 10% aqueous K_2CO_3. $NCCH_2CO_2Et$ (2.5 g.), 4 g. $CO(CH_2CO_2Et)_2$, and 6 drops $EtNH_2$ kept 7 days in 10 ml. alc., the mixture evaporated, the residue (3.2 g.) kept overnight in 20 ml. concentrated H_2SO_4, and poured into H_2O gave 1.4 g. Et 3-ethoxycarbonyl-2,6-dihydroxy-4-pyridylacetate, orange-yellow needles, m. 176.5° (alc.). $CH_2(CN)_2$ (0.35 g.), 0.43 g. Et_2CO, and 2 drops $NHEt_2$ kept 4 days in 2 ml. alc. gave 0.06 g. 2-cyano-3-ethyl-2-pentenonitrile, m. 160-1° (aqueous alc.). Dibenzyl ketone (1.5 g.) after 12 hrs. gave 1.15 g. 3-benzyl-2-cyano-4-phenyl-2-butenonitrile, plates, m. 49.5° (aqueous alc.). Me_2CO and fluorenone gave corresponding products, m. 172-3° and 234°, resp.

IT 53162-08-6P, 1,3,6,8-Copyrinetetrol 114698-11-2P, 1,3,6,8-Copyrinetetrol, 4,5-dinitroso-(?) 116083-61-5P, 1,3,6,8-Copyrinetetrol, dibenzoate
RL: PREP (Preparation)
(preparation of)

RN 53162-08-6 CAPLUS
CN 2,7-Naphthyridine-1,8(2H,7H)-dione, 3,6-dihydroxy- (CA INDEX NAME)



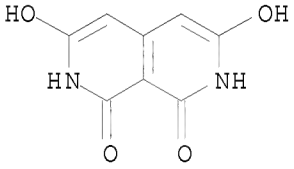
RN 114698-11-2 CAPLUS
CN 2,7-Naphthyridine-1,8(2H,7H)-dione, 3,6-dihydroxy-4,5-dinitroso- (CA INDEX NAME)



RN 116083-61-5 CAPLUS
CN 1,3,6,8-Copyrinetetrol, dibenzoate (6CI) (CA INDEX NAME)

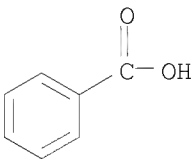
CM 1

CRN 53162-08-6
CMF C8 H6 N2 O4



CM 2

CRN 65-85-0
CMF C7 H6 O2



L7 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1958:88095 CAPLUS
DOCUMENT NUMBER: 52:88095
ORIGINAL REFERENCE NO.: 52:15532a-i
TITLE: 2,7-Naphthyridine derivatives
AUTHOR(S): Birkofer, Leonhard; Kaiser, Christelmargot
CORPORATE SOURCE: Univ. Cologne, Germany
SOURCE: Chemische Berichte (1957), 90, 2933-40
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

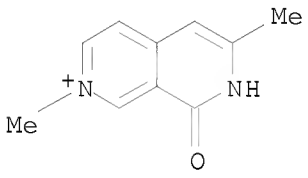
AB N-Methyl-3-aminoformylpyridinium chloride (I) condensed with Me2CO in alkaline solution by the method of Huff (C.A. 41, 2738b), the mixture worked up, and the crude product treated with HCl gave 3,7-dimethyl-1-oxo-1,7-dihydroxy-2,7-naphthyridine.HCl (II), yellowish prisms, m. 320-2° (decomposition). II (2 g.) heated at 290-300°/0.1-0.2 and the sublimate recrystd. (H2O) gave 75-90% 3-methyl-1-oxo-1,2-dihydro-2,7-naphthyridine (III), rods, m. 264° (H2O). I (7.5 g.) in 195 cc. H2O and 195 cc. Me2CO treated with stirring with 24 cc. 7N KOH, kept 12 hrs. at room temperature, treated with 45 cc. concentrated HCl, heated 20 min. in an H2O bath, and evaporated in vacuo, the yellow residue heated 1 hr. at 50° with a little EtOH and kept 24 hrs. at -20°, and the deposit filtered, washed with EtOH, dried, and sublimed at 290°/0.1-0.2 yielded about 20% III. III in MeOH treated with diphenyldisulfimide (IV) gave III.IV adduct, needles, m. 214°. Similarly was prepared the p,p'-dichlorodiphenyldisulfimide derivative of III, m. 175°. III, in MeOH treated with aqueous picric acid gave the picrate of III, yellow needles, m. 234° (decomposition). III refluxed with MeI gave III.MeI, scales, m 309° (decomposition) (aqueous MeOH). III.MeI with AgCl gave II. The recrystn. mother liquors from III basified slightly with aqueous Na2CO3 and evaporated in vacuo, the residue sublimed at 300°/0.1-0.2, the resinous brown precipitate dissolved in H2O, the solution adjusted to pH 4, passed through Amberlite IR-4B, and extracted with CHCl3, the extract evaporated, and the residue distilled gave 2-Me derivative of III, m. 138° (MeOH-Et2O); HCl salt, m. 283-6° (decomposition) (MeOH). III (3 g.) in absolute MeOH treated with excess CH2N2-Et2O, refrigerated 5 weeks, filtered, and evaporated, the residue boiled with H2O, and the aqueous extract worked up gave the N-Me derivative of III, needles, m. 137-8° (picrate, leaflets, m. 217°); the H2O-insol. material (volatile with steam) recrystd. (petr. ether) gave 1-methoxy-3-methyl-2,7-naphthyridine, (V) needles, m. 92° (petr. ether). III (2 g.) and 20 cc. POCl3 heated 1 hr. at 140-5° in a sealed tube, cooled, filtered, and evaporated in vacuo, the residue basified with saturated aqueous Na2CO3 and extracted with CHCl3, and the extract worked up gave an oil-crystal mixture which sublimed at 95-100°/12 yielded 70% 1-chloro-3-methyl-2,7-naphthyridine (VI), leaflets, m. 106° (petr. ether); picrate, m. 157° (MeOH). VI (750 mg.) in a little absolute MeOH added to NaOMe solution, refluxed 1 hr., and evaporated in vacuo, and the residue decomposed with iced H2O, the precipitate dissolved in EtOAc, dried, and evaporated, and the residue recrystd. (petr. ether) yielded V, needles, m. 92°. VI (4.5 g.) heated 2 hrs. at 150° with 15 cc. Et2N(CH2)2NH2, the excess amine distilled, the residue dissolved in dilute aqueous KOH and extracted with Et2O, and the extract worked up gave 1-(Et2N CH2CH2NH) analog of V, yellow viscous oil, b0.012 138-40°; HCl salt, deliquescent crystals, showed in MeOH green fluorescence; dipicrate, yellow leaflets, m. 183° (decomposition)

(MeOH); monopicrate, orange prisms, m. 183-4° (H2O). VI in MeOH hydrogenated over 10 weight-% 1% Pd-CaCO3, filtered, and evaporated, the residue dissolved in H2O, the solution basified with Na2CO3, treated with NaCl, and extracted with CHCl3, and the extract worked up gave 40-50% 3-methyl-2,7-naphthyridine, deliquescent crystals, m. 39°, b0.12 76°; picrate, yellow needles, m. 219-21° (H2O). III (3 g.) in 50 cc. concentrated HNO3 (d. 1.4) heated 8 hrs. on the H2O bath with the occasional addition of a few cc. HNO3 and concentrated at 20 mm., the residue treated with H2O, the precipitate dried and refluxed 20 min. with Ac2O, and the mixture distilled yielded the anhydride of cinchomeronic acid (VII), b12 139-42°, m. 73°, which heated with H2O gave VII, m. 268° (decomposition). The anhydride of VII with EtOH gave the γ-Et ester of VII, prisms, m. 128-31° (EtOAc-ligroine).

IT 112689-01-7P, 7,8-Dihydro-2,6-dimethyl-8-oxocopyrinium iodide
RL: PREP (Preparation)
(preparation of)

RN 112689-01-7 CAPLUS

CN 2,7-Naphthyridinium, 3,7-dimethyl-1-oxo-, iodide (1:1) (CA INDEX NAME)



● I^-

L7 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1957:51897 CAPLUS
DOCUMENT NUMBER: 51:51897
ORIGINAL REFERENCE NO.: 51:9641b-i,9642a-f
TITLE: Structure of gentianine
AUTHOR(S): Govindachari, T. R.; Nagarajan, K.; Rajappa, S.
CORPORATE SOURCE: Presidency Coll., Madras
SOURCE: Journal of the Chemical Society (1957) 551-6
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C.A. 51, 5070c. Powdered Enicostemma littorale (2 kg., from whole plant) made into a paste with 2 l. NH4OH (d. 0.9) and H2O, dried at 30° in the shade, extracted several hrs. with CHCl3, the extract shaken with N H2SO4, the acid extract neutralized with BaCO3 and filtered, the filtrate acidified with AcOH, concentrated, made alkaline with NH4OH, extracted thoroughly with Et2O, and the crude product on evaporation (6-12 g.) crystallized from moist Et2O gave 4-8 g. gentianine (I), m. 82-3°, [α]D30 ± 0° (CHCl3), λ 220, 245, 280 mμ (log ε 4.38, 3.9, 3.2), ν 1719 (αβ-unsatd. δ-lactone), 1634 (conjugated double bond) cm.-1, with no bands in the 1300-1400 cm.-1 (C-methyl) region, no C-Me group by Kuhn-Roth method; HCl salt, m. 169-70° (decomposition); HBr salt, m. 178° (decomposition); HNO3 salt, m. 113° (decomposition); oxalate, m. 123-4°; (+)-tartrate, m. 138°; picrate, m. 123-4°; methiodide, m. 193°. In general the m.p. of the salts agree with those given by Proskurnina, et al. (C.A. 40, 72132; 44, 159d). Treatment with alc. NaOH gave a Na salt from which I was recovered on acidification. I (0.8 g.) in 25 ml. MeOH shaken with H at 55 lb./sq. in. in the presence of PtO2 and the product crystallized from Et2O-petr. ether gave 0.6 g. dihydrogentianine, m. 74-6°, λ 270 mμ (log ε 3.4); picrate, m. 140-2°. I (0.5 g.) ozonized 6 hrs. in 50 ml. dry CHCl3 at 0°, the mixture evaporated in vacuo at 30° and the residue refluxed 1 hr. with 100 ml. H2O, the solution diluted with 100 ml. H2O and 1 ml. AcOH, steam distilled into 200 ml. H2O containing 1.5 g. dimedon, the distillate boiled, filtered hot, and the solution cooled gave HCHO-Me2C6H6O2, m. 187°. Oxidation of 1.45 g. I in 50 ml. Me2CO with 4.4 g. KMnO4 in 300 ml. Me2CO produced 0.94 g. 4-(2-hydroxyethyl)pyridine-3,5-dicarboxylic acid lactone (II), m. 260-2°, λ 265 mμ (log ε 3.1), showing the presence of a vinyl group. Vigorous oxidation of 0.5 g. I in 20 ml. 2N NaOH at 100° with 2 g. KMnO4 in 20 ml. H2O, working up the product, and purifying by passage through Zeo-Karb 315 gave pyridine-3,4,5-tricarboxylic acid, m. 262-4°, also obtained by oxidation of 5-ethyl-4-methylnicotinic acid (III). II (0.94 g.) in 3 ml. H2O containing 0.55 g. KOH evaporated and the salt distilled with 3 g. soda-lime gave crude base (picrate, m. 155-6°), oxidized (100 g.) in 20 ml. H2O containing 1 ml. 2N NaOH at 100° with 0.3 g. KMnO4, the solution filtered, the filtrate and hot H2O washings acidified and evaporated, the residue extracted with boiling alc. yielding isonicotinic acid (picrate, m. 215°), thus establishing the alc. side chain in position 4. Two alternative structures for I given by these degradations were evaluated by synthesis since attempts to decarboxylate the acid from the I dihydro derivative were unsuccessful. The simpler 4-(1-hydroxyethyl)-nicotinic acid lactone (IV) was first synthesized to determine the exptl. conditions. EtCOCH2CO2Et (9 g.), 5 g. NCCH2CONH2, 10 ml. piperidine, and 15 ml. MeOH refluxed 3 hrs., the MeOH evaporated, and the residue in 50 ml. H2O acidified with dilute HCl yielded 3 g. 3-cyano-2,6-dihydroxy-4-ethylpyridine. The nitrile (9 g.) heated 4

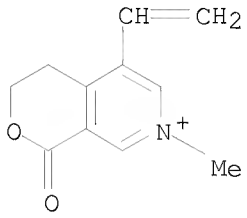
hrs. at 180° with 18 ml. $POCl_3$ in a sealed tube, the cooled mixture poured onto cracked ice, the solution extracted at room temperature with Et_2O, the dried extract evaporated and the crude chloro compound (8 g.) hydrogenated 30 min. at 2 atmospheric in 100 ml. MeOH containing 10 g. KOAc and 0.7 g. $PdCl_3$, the filtered solution evaporated, the residue in 50 ml. H_2O saturated with $NaHCO_3$ and extracted with Et_2O, the dried extract evaporated, and the residue distilled in vacuo gave 3.7 g. 4-ethylnicotinonitrile, b3.5 92-3° (picrate, m. 153-5°), hydrolyzed to 4-ethylnicotinic acid. The acid (0.85 g.) in 6 ml. AcOH containing 2 ml. 30% H_2O heated 3 hrs. at 70°, treated with 2 ml. 30% H_2O, and kept 8 hrs. at 70°, the solution evaporated in vacuo and the residue recrystd. twice from H_2O gave 0.85 g. N-oxide, m. 187-8°, converted by refluxing 4 hrs. in dioxane containing Ac_2O to 4-(1-hydroxyethyl)pyridine acetate (picrate, m. 148-51°) and IV, m. 87-8°, λ 255 mμ (log ε 3.18) (picrate, m. 153°), also obtained by warming 0.5 g. acid into solution with 2 ml. Ac_2O and keeping the mixture overnight at 30°. Similarly, 4,5-diethylnicotinic acid (V) was synthesized from $EtCOCHEtCO_2Et$ (VI). VI (22 g.) shaken 6 days with 40 ml. NH_4OH (d. 0.9), the aqueous layer separated and treated with 16 ml. $NCCH_2CO_2Et$, filtered after standing 4 days at 30°, the residual salt taken up in H_2O and the solution acidified, filtered, and the residue recrystd. from H_2O gave 7 g. 3-cyano-4,5-diethyl-2,6-dihydroxypyridine (VII), m. 186-7° (decomposition). VII (10 g.) heated with 20 ml. $POCl_3$ gave 8 g. chloro compound, hydrogenated in 100 ml. MeOH containing 8 g. KOAc and 0.7 g. $PdCl_4$ to give 3.2 g. 4,5-diethylnicotinonitrile, b. 110° (picrate, m. 144.0-5.5°), which heated 6 hrs. at 140° with 32 ml. 75% H_2SO_4, the iced mixture treated with $Ca(OH)_2$ to pH 5-6, filtered, the filtrate and washings evaporated in vacuo, the residue extracted with alc., the extract evaporated and the residual amino acid sulfate taken up in H_2O and passed through De-Acidite E, the eluate evaporated, and the residue recrystd. from alc.-Et_2O gave 2.5 g. V, m. 115-16°; N-oxide, m. 190-2°. The oxide (0.5 g.) shaken with 2 ml. warm Ac_2O, the dark red solution worked up to give 180 mg. red oily 5-ethyl-4-(1-hydroxyethyl)nicotinic acid lactone; picrate, m. 148-9°, ν 1763 cm.$^{-1}$ (α,β-unsatd. γ-lactone), differing from that of dihydrogentianine picrate, m. 140-2°, ν 1720 cm.$^{-1}$, and so eliminating the structure proposed by P., et al. (loc. cit.), for I. $POCl_3$ (10 ml.) heated 4.5 hrs. at 160° with 5 g. 3-cyano-2,6-dihydroxy-5-ethyl-4-methylpyridine [from $AcCHEtCO_2Et$ (cf. Ruzicka and Fomasir, C.A. 13, 3179)] gave 4.5 g. 3-cyano-2,6-dichloro-5-ethyl-4-methylpyridine, hydrogenated in 50 ml. MeOH containing 0.4 g. $PdCl_4$ and 5.5 g. KOAc to yield 2.5 g. 5-ethyl-4-methylnicotinonitrile, b7 120° (picrate, m. 157-8°), hydrolyzed with 75% H_2SO_4 and worked up to give 5-ethyl-4-methylnicotinic acid (VIII), m. 163-5°. VIII (1 g.) and 3 ml. 40% HCHO heated 24 hrs. at 100° in a sealed tube, excess HCHO removed by steam distillation, the solution concentrated to 5 ml. and extracted with $CHCl_3$–Et_2O, the dried extract evaporated and the Et_2O-washed residue crystallized from MeOH–Et_2O gave 2-(3-carboxy-5-ethyl-4-pyridyl)propane-1,3-diol lactone (IX), m. 168-9°, identical with that obtained by similar treatment of dihydrogentianine, m. 74-6°, synthesized by heating 0.5 g. VIII Na salt 15 hrs. at 100° with 0.3 ml. 40% HCHO and fractionating the

crude product from petr. ether, together with IX. The structure of I is conclusively established and the identity of I from E. littorale and gentianine confirmed. The alkaloid erythricine (C.A. 41, 7676c) may also prove to be identical with I.

IT 117885-38-8
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 117885-38-8 CAPLUS

CN 1H-Pyrano[3,4-c]pyridinium, 5-ethenyl-3,4-dihydro-7-methyl-1-oxo-, iodide (1:1) (CA INDEX NAME)



L7 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1957:51896 CAPLUS
DOCUMENT NUMBER: 51:51896
ORIGINAL REFERENCE NO.: 51:9640b-i,9641a-b
TITLE: Taraxanthin and tarachrome. Stereoisomeric trollixanthins
AUTHOR(S): Eugster, C. H.; Karrer, P.
CORPORATE SOURCE: Univ. Zurich, Switz.
SOURCE: Helvetica Chimica Acta (1957), 40, 69-79
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Pure crystalline taraxanthin (I) (cf. Kuhn and Lederer, C.A. 21, 750) has been isolated from Bundner Rheintal summer crop yellow balsam (Impatiens noli-tangere) by a modification of the procedure of K. and L. Shade-dried blossoms (5500) (45.5 g.) warmed gently with C6H6, kept overnight and decanted, the extraction repeated and the material dried in vacuo at 40°, milled and again extracted with C6H6, the combined exts. evaporated in vacuo (N atmospheric), the viscous oily residue taken up in 70 cc. C6H6, treated with 6.5 g. KOH in 50 cc. alc. and some petr. ether, the mixture kept 8 hrs. at room temperature and warmed 45 min. at 70°, the cooled mixture diluted with H2O and extracted several times with Et2O, the washed and dried extract filtered and evaporated, the pigment resin distributed between 50 cc. MeOH and 70 cc. petr. ether (b. 30-60°), filtered from precipitated I, the epiphase extracted with 50 cc. 90% MeOH, the combined MeOH exts. evaporated, taken up in MeOH and centrifuged at 3500 r.p.m. with addition of petr. ether, the precipitate again precipitated by centrifugation from MeOH and petr. ether, the powdery product taken up in C6H6, filtered and the filtrate evaporated in vacuo, the residue dried at 40° in vacuo, combined with precipitated I and extracted with boiling C6H14, the insol. residue crystallized from MeOH, the crude pigment (57.7 mg., m. 175.0-7.5°) recrystd. from MeOH, the coppery-shining prisms (38.9 g., m. 180.5-1.5°) recrystd. slowly from C6H6 and C6H12 gave 32.0 g. reddish granular I, C40H66O4, m. 183.5-4.0°, λ 501.5, 469, 442 mμ (in CS2); 48.5, 455, 428.5 mμ (ε 132,300, 138,600, 91,700, in C6H6). I is isomeric with violaxanthin (II), λ 483, 453.5, 428 mμ (ε 128,400, 134,400, 88,500, in C6H6) and trollixanthin (III), λ 482, 454, 427 mμ [ε 121,800, 127,700, 84,400, in C6H6, trans form (IIIa)]. I differs from II which gives a very stable dark blue salt with 20% HCl. On shaking in Et2O with 25% (or stronger) HCl pure I gives a faint pos. blue coloration indicative of the presence of an epoxy grouping or its rearrangement product. The combined mother liquors from crystallization of I taken up in 50 cc. CHCl3, the red solution treated with 5 cc. 0.012N HCl in CHCl3, after 90 sec. the green solution shaken with excess aqueous NaHCO3, the bright red mixture washed with H2O, filtered through an adsorbent cotton column, and the filtrate evaporated in vacuo gave a residue, λ 459.5, 435 mμ (in C6H6). The residue in C6H6 chromatographed over a 4:1 CaCO3-Celite column (7.4 + 22 cm.), developed with 1 l. C6H6-petr. ether and 550 cc. C6H6, the egg-yellow zone eluted with Et2O-MeOH, the eluate evaporated and the pigment taken up in 2 cc. C6H6, the solution treated with excess petr. ether and filtered, the yellow substance recrystd. from MeOH at -15°, and the yellow microcryst. product twice recrystd. from MeOH at -20° and again from MeOH at 0° gave tarachrome (IV), m. 154-64°, λ, 460, 434 mμ (in C6H6); 478, 449 mμ (in CS2). Further purification by chromatography on 4:1 ZnCO3-Celite from C6H6 with 15% Me2CO3 by elution of the egg-yellow zone with Et2O-MeOH and crystallization from

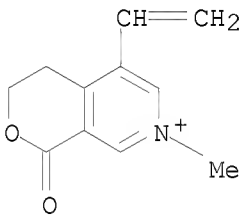
MeOH yielded 3 mg., m. 162-8°, λ 460, 431.5, 407.5 mμ (ε 118,000, 119,400, 74,900), indicative of a sterically nonhindered all-trans polyene system, and practically congruent with the curves of trollichrome (V), flavoxanthin, and chrysanthemaxanthin. The chromatograms gave no evidence of an isomeric mixture such as occurs in the acid rearrangement of xanthophyll epoxide (VI). I liberates 3 moles CH_4 in Zerevitinov active-H determination and consumes 10.7 moles H in hydrogenolysis.

I is regarded as an hydroxylated VI of which IV is the furanoid rearrangement product. Pure I (16.6 mg.) in 13 cc. $CHCl_3$ treated with 0.012N HCl in $CHCl_3$, shaken 90 sec. later with excess $NaHCO_3$ solution, the orange solution worked up to a resin, taken up in Et_2O and evaporated (N atmospheric), and the crystalline residue recrystd. from C_6H_6 and MeOH gave fine yellow leaflets of IV, m. 162-8°, $C_{40}H_{56}O_4$. Various specimens of previously isolated III, m. 143-5°, 155-6°, and 199°, were reexamd. to check their nonidentity with pure I, since all were rearranged to give the same V, m. 206°. These various forms consist of IIIa, m. 199°, λ 482, 454, 427 mμ (ε 121,800, 127,700, 84,400, c 1.07 + 10-5 m., in C_6H_6), cis-III (IIIb), m. 143-5°, λ 481, 456, 430 mμ (ε 50,900, 74,000, 64,000, c 1.182 + 10-5, in C_6H_6), and a difficultly separated mixture of IIIa and IIIb. All attempts to invert the cis form to the all-trans form gave only unchanged IIIb, V, or decomposition products. The occurrence of IIIb in some specimens of Trollius europaeus (mountain globe flower) and of IIIa in others may depend on the time of harvesting (cf. Zechmeister and Schroeder, C.A. 37, 11529).

IT 117885-38-8
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 117885-38-8 CAPLUS

CN 1H-Pyrano[3,4-c]pyridinium, 5-ethenyl-3,4-dihydro-7-methyl-1-oxo-, iodide (1:1) (CA INDEX NAME)



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=> FIL STNGUIDE

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	80.62	439.41

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-11.20	-11.20

FILE 'STNGUIDE' ENTERED AT 10:41:12 ON 03 DEC 2008

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Nov 21, 2008 (20081121/UP).